Mrunal’s part of the report:

**Chemical Informational Analysis**

The mechanism that will be utilized in this plant’s production of propionic acid is the carbonylation of ethylene to produce propionaldehyde which will then further be oxidized to produce propionic acid. The chemical equations governing this process are as follows:

As shown above, the process will require a 1:1:1 ratio of carbon monoxide to hydrogen gas (which will be the composition of the syngas fed in from team Foxtrot) to ethylene. Both initial feed flow rates will be determined in the material balance by starting with the amount produced per year and working backwards using the conversion rates of the two reactors. Similarly, the air flow rate that will be used to obtain the oxygen needed for the second reaction will be determined using the same process.

The first reaction is set to take place under the influence of a nickel carbonyl. The nickel based catalyst is a highly toxic substance that has a permissible exposure limit of 0.001 ppm, or 1 ppb1. As the acid that is being produced will be used as food preservatives2 one of the major concerns of the project is the recovery or, at the very least, the destruction of this particular catalyst so that it does not contaminate the food we and animals consume. As for the process itself, the nickel carbonyl catalyst is poisoned by 5 ppm/6 hrs of sulfur3. Since the syngas being fed into the plant is obtained from the combustion of coal, the presence of sulfur is a real issue that needs to be addressed. Also if it is determined that destruction of the catalyst is the only option then the price of the catalyst becomes a major expense as it would need to be fed in constantly, with the commodity price for nickel carbonyl at $14-17/lb4.

The second reaction is a rapid oxidation of the propionaldehyde that was synthesized in the first reactor. This reaction will utilize a cobalt ion as the catalyst which is to be obtained by dissolving a cobalt halide in water. The known poisons of the cobalt catalyst is potassium carbonate5, however due to the lack of potassium in the entire system there is no real worry for the poisoning of this catalyst.

**Material and Energy Balance**

The material and energy balance is as follows based on the design specification of 33000 tons per year of propionic acid, also with the assumptions that both reactors have a 99.5% conversion rate, 337 operating days per year and the separator completely removes the aldehyde from the reactants.

Material Balance

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Stream Number | 1 | | 2 | | 3 | | 4 | |
| From |  | | ETHCOMP | | COOLERET | |  | |
| To | ETHCOMP | | COOLERET | | REACT1 | | REACT1 | |
| Stream Phase | Vapor | | Vapor | | Vapor | | Vapor | |
| Total Mass Rate #/hr | 3120 | | 3120 | | 3120 | | 3341 | |
| Composition | #/hr | wt% | #/hr | wt% | #/hr | wt% | #/hr | wt% |
| Ethylene | 3120 | 100.00 | 3120 | 100.00 | 3120 | 100.00 | 0 | 0.00 |
| Carbon Monoxide | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 3116 | 93.27 |
| Hydrogen Gas | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 225 | 6.73 |
| Propionaldehyde | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 |
| Propionic Acid | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 |
| Oxygen | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 |
| Nitrogen | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 5 | | 6 | | 7 | | 8 | | 9 | |
| REACT1 | | DECOMPRE | | FLASH | | RECCOMP | | COOL | |
| DECOMPRE | | FLASH | | RECCOMP | | COOL | | REACT1 | |
|  | |  | |  | |  | |  | |
| 6462.14 | | 6462.14 | | 32.14 | | 32.14 | | 32.14 | |
| #/hr | wt% | #/hr | wt% | #/hr | wt% | #/hr | wt% | #/hr | wt% |
| 15.52 | 0.24 | 15.52 | 0.24 | 15.52 | 48.29 | 15.52 | 48.29 | 15.52 | 48.29 |
| 15.5 | 0.24 | 15.5 | 0.24 | 15.5 | 48.23 | 15.5 | 48.23 | 15.5 | 48.23 |
| 1.12 | 0.02 | 1.12 | 0.02 | 1.12 | 3.48 | 1.12 | 3.48 | 1.12 | 3.48 |
| 6430 | 99.50 | 6430 | 99.50 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 |
| 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 |
| 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 |
| 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 10 | | 11 | | 12 | | 13 | | Stream Number |
| FLASH | | ALDHEAT | |  | | OXIDIZE | | From |
| ALDHEAT | | OXIDIZE | | OXIDIZE | |  | | To |
|  | |  | | Vapor | |  | | Stream Phase |
| 6430 | | 6430 | | 7629 | | 14065 | | Total Mass Rate #/hr |
| #/hr | wt% | #/hr | wt% | #/hr | wt% | #/hr | wt% | Composition |
| 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | Ethylene |
| 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | Carbon Monoxide |
| 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | Hydrogen Gas |
| 6430 | 100.00 | 6430 | 100.00 | 0 | 0.00 | 32.15 | 0.23 | Propionaldehyde |
| 0 | 0.00 | 0 | 0.00 | 0 | 0.00 | 8160 | 58.02 | Propionic Acid |
| 0 | 0.00 | 0 | 0.00 | 1765 | 23.14 | 8.825 | 0.06 | Oxygen |
| 0 | 0.00 | 0 | 0.00 | 5864 | 76.86 | 5864 | 41.69 | Nitrogen |

Energy Balance

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | 1 | 2 | 3 | 4 |
| Molar Enthalpy (BTU/#) | 804 | 1194 | 1042 | -1351 |
| Enthalpy Flow (BTU/hr) | 2.5E+06 | 3.7E+06 | 3.3E+06 | -4.5E+06 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 5 | 6 | 7 | 8 | 9 |
| -1130 | -1130 | -818 | 548 | 177 |
| -7.3E+06 | -7.3E+06 | -2.6E+04 | 1.8E+04 | 5.7E+03 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 10 | 11 | 12 | 13 |  |
| -1620 | -1518 | 0 | -2763 | Molar Enthalpy (BTU/#) |
| -1.0E+07 | -9.8E+06 | -3.3E+03 | -3.9E+07 | Enthalpy Flow (BTU/hr) |

|  |  |  |  |
| --- | --- | --- | --- |
| Total Enthalpy (BTU/hr) | -6.87E+07 | | |
|  |  |  |  |
| Enthalpy of CSTR1 (BTU/hr) | -6.05E+06 | | |
| Enthalpy of CSTR2 (BTU/hr) | -2.91E+07 | | |

(these values are subject to change as the project moves forward)